|   | Benzoic acid, 4-methoxy- |   |
|---|--------------------------|---|
| 1 | 00-09-4   DTXSID405920   | 5 |
|   |                          |   |

## **Model Performance**

|        | n .    |
|--------|--------|
| Model  | I )ata |
| Widdei | Data   |
|        |        |

## Weighted KNN model

| 5-fold CV | 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |  |
|-----------|-----------------|------|----------------|------|------------|--|
| Q2        | RMSE            | R2   | RMSE           | R2   | RMSE       |  |
| 0.85      | 0.69            | 0.86 | 0.67           | 0.86 | 0.78       |  |

## Model Results

Predicted value: 2.18

Global applicability domain: Inside

Local applicability domain index: 7.04e-01

Confidence level: 6.71e-01

## Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 3-methoxy-

Measured: 2.02 Predicted: 2.18 Image not found

Ethyl salicylate Measured: 2.95 Predicted: 2.38 Image not found

Benzoic acid, 4-methoxy-

Measured: 1.96 Predicted: 2.18

Image not found

3-Methoxyphenylacetic acid

Measured: 1.50 Predicted: 2.04 Image not found

Ethylparaben
Measured: 2.47
Predicted: 2.13